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United States Environmental Protection Agency
Washington, DC 20460

ORIGINAL

Document Description	Date
SAT RPT P-02-238-239	Feb. 11/02

[redacted]

EPA Form 7740-9 (rev. 10/92) Previous edition is obsolete

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

[redacted]

Case #: P-02-0238-239	**DCN:**
SAT Date: 1/25/02	**SAT Chair:** V. Nabholz

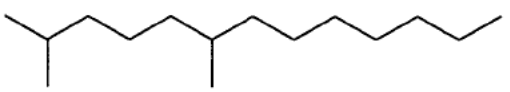
Submitter: Shell Chemical Company

Chemical Name:

Pentadecane, branched

CAS RN: 362520-89-6	**Trade Name:** Hydrocarbon blend stock 150B

Structure



[redacted]

Molecular Formula:	$C_{15}H_{32}$		
Molecular Wt. 212	**WT%<500:**	**WT%<1000:**	
MP:	**BP:** 250	**Eq. Wt:**	
H2O Sol (g/L): 3x10-6	**V.P.** 0.044		
Max. Prod. Volume (kg/yr): 5239000	**Physical State:** Liquid		

USE:

Component in drilling fluid (80%) and fuel (20%).

Related Case Numbers	Case Role	Related Case Numbers	Case Role
[redacted]		[redacted]	

Focus **Date:** FEB 7 2002 **Results:** DROP – HPV

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98 [redacted]

Case #: P-02-0239	**DCN:**
SAT Date: 1/25/02	**SAT Chair:** V. Nabholz

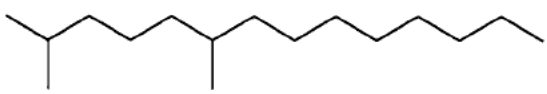
Submitter: Shell Chemical Company

Chemical Name:

Hexadecane, branched

CAS RN: 362520-79-4	**Trade Name:** Hydrocarbon blend stock 150B

Structure



[redacted]

Molecular Formula: $C_{16}H_{34}$

Molecular Wt. 226	**WT%<500:**	**WT%<1000:**
MP:	**BP:** 257	**Eq. Wt:**
H2O Sol (g/L): 1.2x10-6	**V.P.** 3x10-2	
Max. Prod. Volume (kg/yr): 9700000	**Physical State:** Liquid	

USE:

Component in drilling fluid (80%) and fuel (20%).

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus Date: FEB 7 2002 Results: DROP – HPV

STRUCTURE ACTIVITY TEAM REPORT 25 January 2002 [redacted]

CASE NUMBERS: **P02-0238 (C15) and 0239 (C16)**
NOTE: Branching is a mean of 1.6 methyls per alkyl

RELATED CASES: [redacted]

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL:	1-2	1

KEYWORDS: LUNG, IRR-MM

SUMMARY OF ASSESSMENT:

FATE: MW212 and 226
liquid with mp = -9 °C (P)
log Kow = 8.4 and 8.9 (ClogP), 7.6 and 8.0 (EPI)
S = 0.003 to 0.004 mg/L and 0.001 mg/L at 20 °C (P)
vp = 0.044 and 0.03 mm Hg or torr at 25 °C (P);
bp = 250 and 260 °C (P);
H = 22 (P);
log Koc => 4.5 (P);
log fish BCF => 2.5 (P);
POTW removal = 99% via sorption and stripping
time for complete ultimate aerobic biodegradation = weeks to months;
sorption to soils and sediments = strong;
volatilization from rivers = 1 hours and from lakes = 6 days;
atmospheric oxidation half-life = 6.8 hours via OH radical
PBT Potential: P2B1T1
*CEB FATE: migration to ground water = slow

HEALTH: Absorption is poor all routes based on analogs;

test data for the C16 analog, [redacted] were:
rat acute oral LD50 > 46.4 mL/kg;
mild skin irritation in rabbits
mild eye irritation in rabbits;

test data for the C20 analog, [redacted], were:
Ames test negative
mouse micronucleus ip was negative
rat 28-d oral-gavage NOAEL = 1 g/kg/d (highest dose tested)

concern for lung toxicity if inhaled and irritation to mucous membranes;

low to moderate concern for toxicity;
*CEB HEALTH: Exposures to humans: inhalation; XB: No testing desired.

ECOTOX: Submitted test data were for an analog whose chemical identity was unknown;

Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	=	*	P
daphnid 48-h LC50	=	*	P
green algal 96-h EC50	=	*	P
fish chronic value	=	*	P
daphnid ChV	=	*	P
algal ChV	=	*	P

Predictions are based on SARs for neutral organic chemicals; SAR chemical class = alkane-C15 and C16; MW212 and 226; log Kow = 8.4 and 8.9 (ClogP); pH7; effective concentrations based on 100% active ingredients and nominal concentrations; hardness <180.0 mg/L as CaCO3; and TOC <2.0 mg/L;
low concern for toxicity;

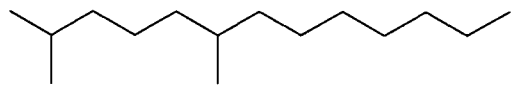
assessment factor	=	10.0
concern concentration	=	*

*CEB ECOTOX: No releases to water; XB: No testing desired.

SAT Co-chairperson: Vince Nabholz, 564.8909

NCSAB SAT REPORT		CBI? (Y/N):
PMN:	P-02-0238	CAS RN: 362520-89-6
Chemical Name: Pentadecane, branched 2387		Analogs:
		Production Volume: 5239000.00

Structure:



Use:

Component in drilling fluid (80%) and fuel (20%).

Formula: $C_{15}H_{32}$	Eq Wt:			
Mol Weight: 212.42	Wt%<500:			Wt%<1000
MP:		BP:	250	VP: 0.044
H2O Sol (g/L): 3x10-6	Physical State: Liquid			Log P: 7.63 EPI 8.37 CLOGP

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	*		
Daphnid 48-h	*		
Algal 96-h	*		
Fish ChV	*		
Daphnid ChV	*		
Algal ChV	*		
BCF			

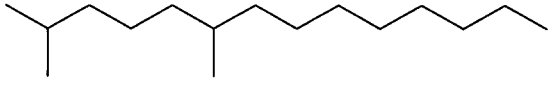
CHEMICAL CLASS:	SAR: alkane - C15
ECOTOX CONCERN: H M (L)	CONCERN CONCENTRATION: *
DATE: 1/25/02	ASSESSOR:

CHEMICAL: Unknown 11:27:47 01/24/:2
MOL WT : 212.42
MOL FOR: C15H32
SMILES : CC(C)CCCC(C)CCCCCCC
ISOC-ID: AA-A-AAAA-A-AAAAAAA
FRAG-ID: _____
H-COUNT: 31_3_2221_3_2222223

Class	Type	Contribution Description	Comment	Value
ISOLATING	CARBON	15 Aliphatic isolating carbon(s)		2.925
EXFRAGMENT	BRANCH	2 chain and 0 cluster branch(es)	(Chain)	-0.260
EXFRAGMENT	HYDROG	32 Hydrogen(s) on isolating carbons		7.264
EXFRAGMENT	BONDS	13 chain and 0 alicyclic (net)		-1.560
SCREEN	NOTE	Very high value unrealistic in nature		0.000
RESULT	v3.3	Very high LogP unrealistic in nature	ESTIMATE	8.369

NCSAB SAT REPORT		CBI? (Y/N):
PMN:	P-02-0239	CAS RN: 362520-79-4
Chemical Name: Hexadecane, branched 2387		Analogs:
		Production Volume: 9700000.00

Structure:



Use:

Component in drilling fluid (80%) and fuel (20%).

Formula: $C_{16}H_{34}$		Eq Wt:		
Mol Weight:	226.45	Wt%<500:		Wt%<1000
MP:		BP:	257	VP: 3x10-2
H2O Sol (g/L):	1.2x10-6	Physical State:	Liquid	Log P: 8.0 EPI

Endpoint (mg/L)	Est. Value	Meas. Value	Comments 8.9 CLOGP
Fish 96-h	*		
Daphnid 48-h	*		
Algal 96-h	*		
Fish ChV	*		
Daphnid ChV	*		
Algal ChV	*		
BCF			

CHEMICAL CLASS:				SAR: alkane - C16
ECOTOX CONCERN	H	M	(L)	CONCERN CONCENTRATION *
DATE 1/25/02				ASSESSOR:

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE FEB 1 2002

	ATTENDEES	SIGNATURE
CHEMISTRY		
___	Paul Bickart	
___	Diana Darling	D. Darling
___	Rich Engler	
___	Greg Fritz	
___	Daniel Lin	
___	Kathy Schechter	
___		
___		
ENVIRONMENTAL FATE		
___	Bob Boethling	
___	David Lynch	
✓	Gary Thom	
___		
___		
HEALTH		
✓	Katherine Anitole	Katherine Anitole
✓	Michael Cimino	Michael C Cimino
✓	Leonard Keifer	Leonard Keifer
✓	David Lai	David Lai
___	Jim Murphy	
___	Deborah Norris	
✓	Ronald Ward	Ronald Ward
___	Yin Tak Woo	
___		
___		
___		
ENVIRONMENTAL EFFECTS		
✓	Gordon Cash	Gordon Cash
___	Vince Nabholz	
___	Maggie Wilson	
___		
SAT CHAIRPERSON/OTHER		
___	Rebecca Jones	
✓	Leonard Keifer	
✓	Vince Nabholz	
___		
___		